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Dynamic NMR Study of the Effect of Solvent on Parameters of Ternary Conformational Equilibrium in 12-Hydroxydibenzo[d,g][1,3]dioxecins

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Abstract

The effect of solvent on the thermodynamic parameters of ternary conformational equilibrium in cyclic systems was studied by dynamic NMR. 12-Hydroxydibenzo[d,g][1,3]dioxecin and its alkyl derivatives, 12-hydroxy-12-methyldibenzo[d,g][1,3]dioxecin and 12-hydroxy--2-ethyldibenzo[d,g][1,3]dioxecin, were chosen as models. The free energies and enthalpies of the conformational equilibria boat-chair-a-boat-chair-e in 2-hydroxydibenzo[d,g][1,3]dioxecin and boat-chair-a-twist-boat and boat-chair-e-twist-boat in 12-hydroxy--2-methyldibenzo[d,g][1,3]dioxecin and 12-hydroxy-12-ethyldibenzo[d,g][1,3]dioxecin in carbon disulfide, toluene, chloroform, methylene chloride, and acetone were determined. The contribution of the intrinsic temperature dependence of the dielectric permittivity of the solvent to the observed enthalpies was taken into account. The experimental data showed that the dipole approximation does not provide adequate description of the solvation effects of solvents on the conformational equilibrium in 12-hydroxydibenzo[d,g][1,3]dioxecin and its alkyl derivatives.